

# Orderings and renormalization-group flows of a stacked frustrated triangular system in three dimensions

A. Nihat Berker

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Gary S. Grest and C. M. Soukoulis

Exxon Research and Engineering Company, Annandale, New Jersey 08801

Daniel Blankschtein and M. Ma

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Two distinct partially ordered phases have been revealed by the Landau–Ginzburg–Wilson and Monte Carlo studies of the stacked frustrated triangular Ising model. These two types of order, occurring consecutively as temperature is lowered, and an observed shifting between equivalent ordered phases at a given temperature can be explained by a physical interpretation of the expected global renormalization-group flows in temperature and sixfold symmetry-breaking field acting on the two-component order parameter. New Monte Carlo data are presented, which confirm long-range order and a previous prediction of the above interpretation. The transition from the paramagnetic phase is in the  $XY$  universality class, whereas the transition between the ordered phases appears to be a sixfold symmetry-breaking flop.

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The Ising spin system constructed by stacking antiferromagnetic triangular lattices has an infinite ground-state degeneracy due to the fully frustrated  $xy$  planes, but is a candidate for finite-temperature ordering due to the stabilizing  $z$  direction. Indeed, Landau–Ginzburg–Wilson (LGW) and Monte Carlo analyses have revealed two ordered phases.<sup>1</sup> In the low-temperature phase, one sublattice is fully ordered and, oppositely, two sublattices are partially ordered. In the intermediate-temperature phase, two sublattices are fully and oppositely ordered, and one is disordered. The various ordering phenomena exhibited by this system can be coherently explained and predicted by postulated global renormalization-group flows. One is led, in this process, to an interesting comparison between the global flows, in two and three dimensions, of the six-state clock model, to which the present system is related by LGW theory.

The Hamiltonian of the model is

$$\mathcal{H} = J \sum_{\langle ij \rangle}^{xy} s_i s_j - J' \sum_{\langle ij \rangle}^z s_i s_j, \quad (1)$$

where  $J, J' > 0$ ,  $s_i = \pm 1$ , and  $\langle ij \rangle$  indicates summation over nearest-neighbor pairs in the  $xy$  plane or along the  $z$  direction. The possible onset of order can be deduced from LGW theory.<sup>2</sup> The Hamiltonian is Fourier transformed,

$$\mathcal{H} = \sum_{\mathbf{q}} \left\{ J \left[ \cos(q_x) + 2 \cos(q_x/2) \cos(\sqrt{3}q_y/2) \right] - J' \cos(q_z) \right\} s(\mathbf{q}) s(-\mathbf{q}), \quad (2)$$

where the sum is over a hexagonal Brillouin zone. Although the summand appears diagonalized, the many-body problem is not truly solved, since the hard-spin condition  $s_i = \pm 1$  translates into the constraint  $N^{-1} \sum_{\mathbf{k}} s(\mathbf{k}) s(\mathbf{q} - \mathbf{k}) = \delta(\mathbf{q})$ . A basic hypothesis is that this constraint is not conserved under rescaling and therefore is irrelevant to asymptotic criticality. Thus, the mode(s) with the lowest energy  $J(\mathbf{q})$  is predicted to become critical as temperature is lowered from the disordered phase, unless preempted by a strongly first-order transition. Here, these are the two degenerate modes  $\mathbf{Q}_{\pm}$

$= (\pm 4\pi/3, 0, 0)$ , covering the six corners of the Brillouin zone via reciprocal lattice vectors. A two-component ( $n = 2$ ) order parameter is thus deduced.<sup>1</sup> The LGW Hamiltonian is constructed in terms of the near-critical modes,  $s(\mathbf{Q}_{\pm} + \mathbf{q}) = m(\mathbf{q}) \exp[\pm i\theta(\mathbf{q})]$ ,  $|\mathbf{q}| \ll 1$ , by noting all possible invariants under the symmetries of the system, at each consecutive order:

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{q}} (r + q^2) m^2 + u_4 \sum_{\mathbf{q}} m^4 + u_6 \sum_{\mathbf{q}} m^6 + v_6 \sum_{\mathbf{q}} m^6 \cos(6\theta), \quad (3)$$

where  $\sum_p$  signifies summation over  $p$  momentum arguments which add to zero. This is the Hamiltonian of an  $XY$  ( $n = 2$ ) model with sixfold symmetry breaking, also known as the continuum six-state clock model.<sup>3</sup>

The microscopic configuration of the ordered phases is obtained<sup>1</sup> by Fourier transforming the modes which minimize Eq. (3). For  $v_6 < 0$ , the minimal angles are  $\theta = 0, \pi/3, 2\pi/3, \dots$ , assigning the magnetizations  $(M, -M/2, -M/2)$  to the three sublattices of the triangular  $xy$  planes [Fig. 1(a)], with translational symmetry along the  $z$  direction. For  $v_6 > 0$ , these angles are shifted by  $\pi/6$ , assigning the sublattice magnetizations  $(M, -M, 0)$  shown in Fig. 1(b). Each of these two ordered phases is sixfold degenerate, as seen by the six minimal angles or, correspondingly, by up-down symme-

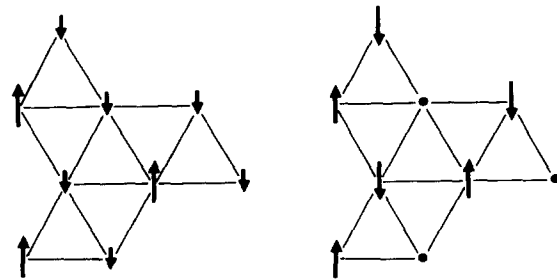


FIG. 1. The  $(M, -M/2, -M/2)$  and  $(M, -M, 0)$  phases, respectively occurring at low and intermediate temperatures.

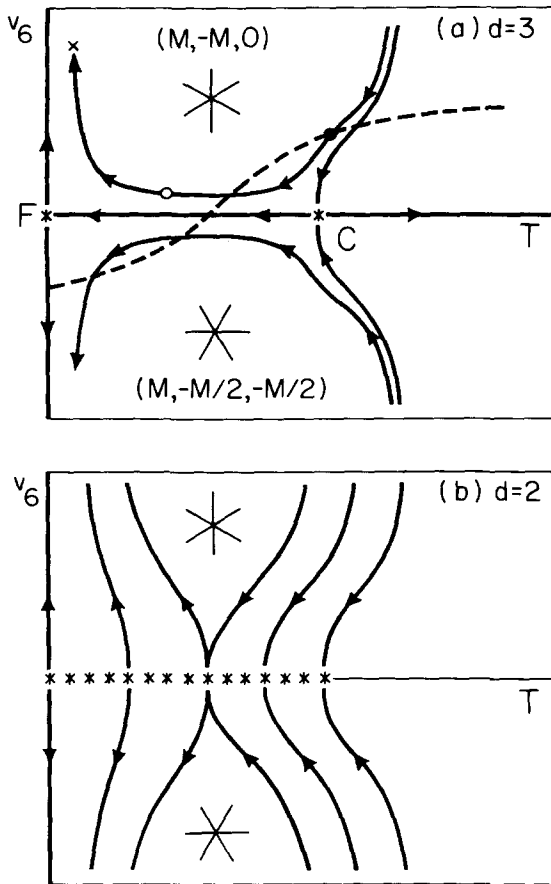


FIG. 2. Postulated global renormalization-group flows. The quantitative rendition of the original Hamiltonian (1) by the LGW Hamiltonian (3) cannot be unambiguously evaluated. In hindsight of the Monte Carlo results, the schematic dashed line in Fig. 2(a) must be the locus of initial conditions, explaining the transition between the two ordered phases as a spin flop.

try  $M \rightarrow -M$  and the three ways of singling out one sublattice.

Both types of ordering raised by LGW theory have been seen by Monte Carlo simulation. The  $(M, -M/2, -M/2)$  and  $(M, -M, 0)$  phases occur respectively at low and intermediate temperatures. The first results<sup>1</sup> were obtained on  $15 \times 15 \times L$  lattices, where  $L = 4, 8, 12$  is the number of layers, with periodic boundary conditions. These results have been further developed with recent runs on larger lattices, to be described below. But first, a peculiar shift phenomenon will be discussed.

In the intermediate-temperature phase, which we first studied rather extensively with the lattice sizes quoted above, the system moved readily between the six degenerate ordered phases, for example shifting from the  $(M, -M, 0)$  phase to the  $(M, 0, -M)$  phase. For these lattice sizes, such shifts occurred at the time scale of a few hundred Monte Carlo steps per spin (MCS). To understand this phenomenon, we consider the global renormalization-group flow diagram [Fig. 2(a)]. To first order in  $\epsilon = 4 - d$ ,  $v_6$  is irrelevant at the transition from the disordered phase.<sup>1</sup> Accordingly, the phase boundary coincides with the flow arriving to the isotropic  $XY$  ( $v_6 = 0$ ) fixed point  $C^*$ , which therefore dictates the critical properties. By contrast, the strong-coupling (zero-temperature) fixed point  $F^*$  is a first-order fixed point

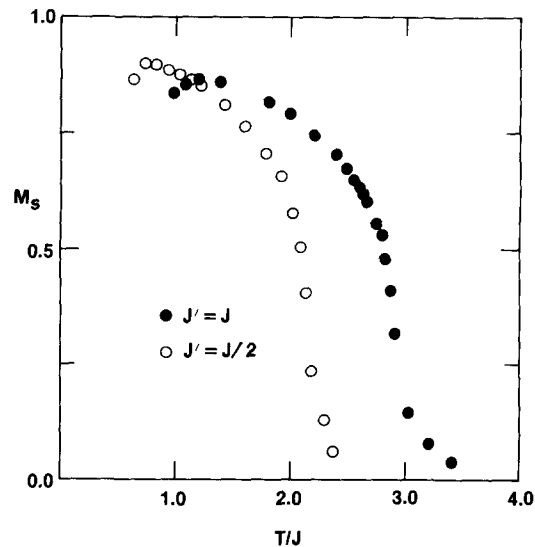


FIG. 3. Staggered magnetization  $M_s$  for  $J' = J/2$  (○) and  $J' = J$  (●). Results for  $J' = J$  are from a  $30 \times 30 \times 15$  system, while those for  $J' = J/2$  are from a  $24 \times 24 \times 15$  system. At the lowest  $T$ , results varied too widely from run to run to be quantitatively reliable, reflecting kinetic effects.

controlling the flop line between the two types of sixfold ordered phases of  $v_6 \geq 0$ . It is necessary for  $F^*$  to be unstable in the  $v_6$  direction, with eigenvalue exponent equal to spatial dimensionality.<sup>4</sup> The  $v_6$  component of the flows must reverse direction somewhere between  $F^*$  and  $C^*$ .

The situation can be instructively compared with the similar two-dimensional ( $d = 2$ ) case.<sup>3</sup> The  $v_6$  flows again reverse direction, but here the  $T < T_c$  axis is a continuum of fixed points [Fig. 2(b)]. Thus, the intermediate-temperature flows actually reach a segment of this fixed line, so that the region of these flows is distinct as an algebraically ordered phase.<sup>3,5</sup> Each such flow constitutes a line of "equicriticality," e.g., constant critical exponent  $\eta$ . By contrast, in  $d = 3$ , where the fixed line is replaced by the  $C^*$  to  $F^*$  flow, the intermediate-temperature flows, while approaching  $v_6 = 0$ , relentlessly drift to low temperatures. They can never reach  $v_6 = 0$ , since each consecutive step in that direction becomes smaller, and eventually enter the low-temperature region where  $v_6$  is amplified. They veer off from  $F^*$  and run away to infinite  $v_6$ . This global picture is postulated from the continuity of the flows, i.e., the analyticity of the recursion relations.

The statistical mechanics of a thermodynamic system involves following to the bitter end the renormalization-group trajectory determined by the initial parameters of the system. Thus, in  $d = 2$ , an intermediate-temperature system is asymptotically equivalent to the isotropic  $XY$  model, e.g., in the algebraic decay of the long-distance correlations. Similarly, in  $d = 3$ , an initial condition in either ordered phase renormalizes to an infinite  $|v_6|$ , meaning that the thermodynamic system is pinned into one of the six clock directions. The situation is different for finite systems, however. Only a finite number of rescalings can be carried out, until a single degree of freedom is left determining the overall properties of the system. That is, a finite flow segment, depending on the system size, is taken from the initial condition. Then, a one-body calculation is done at the terminal condition. Ap-

plying this procedure<sup>6</sup> to Fig. 2(a), consider the initial condition represented by a black circle. For the finite system subjected to Monte Carlo simulation, the terminal condition could be the open circle, with very small  $|v_6|$ . Then, the system would undergo overall shifts between the six clock directions, explaining our observations. Conversely, a larger system would reach, from the same initial condition, a terminal point further along the trajectory, shown with a cross in Fig. 2(a). The large terminal value of  $|v_6|$  would virtually eliminate any shifts.

This earlier prediction<sup>1</sup> has now been confirmed. We have now extended the Monte Carlo simulations to  $L' \times L' \times L$  lattices with  $L' = 15, 24, 30$  and  $L = 4, 8, 12, 15$ . The shifts, which were at the time scale of a few hundred MCS for the  $15 \times 15 \times 12$  lattice, occur at a time scale of thousands of MCS for the  $30 \times 30 \times 15$  lattice, in agreement with the picture above. This indicates the system has true long-range order in the thermodynamic limit. Figure 3 shows the staggered magnetization  $M_s = (\langle s_i^{(1)} \rangle - \langle s_j^{(2)} \rangle)/2$ , where the sublattices were relabelled by decreasing magneti-

zation. Between 1000 and 2000 MCS were taken at each temperature, with data thrown out during shifts between the six degenerate phases. A sharp onset of  $M_s$  vs  $T$  is obtained, as expected for a second-order phase transition.

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